Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 07:13 PM JST

PDB ID	:	6A22
Title	:	Ternary complex of Human ROR gamma Ligand Binding Domain With Compound T.
Authors	:	Noguchi, M.; Nomura, A.; Doi, S.; Yamaguchi, K.; Adachi, T.
Deposited on	:	2018-06-08
Resolution	:	2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

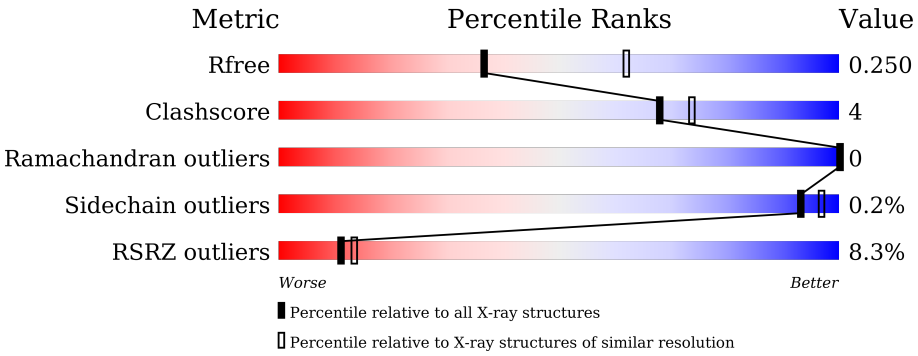
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	258	7% 81% 8% 10%
1	C	258	9% 80% 8% 12%
1	E	258	4% 74% 13% • 12%
1	G	258	8% 79% 9% 12%
2	B	22	18% 64% 5% 32%
2	D	22	9% 41% 9% 5% 45%

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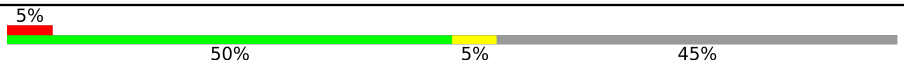
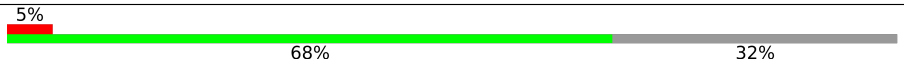
Mol	Chain	Length	Quality of chain
2	F	22	
2	H	22	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8079 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nuclear receptor ROR-gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	1	0
			1887	1198	338	336	15			
1	C	228	Total	C	N	O	S	0	0	0
			1856	1177	334	331	14			
1	E	228	Total	C	N	O	S	0	1	0
			1864	1182	335	333	14			
1	G	228	Total	C	N	O	S	0	0	0
			1857	1178	334	331	14			

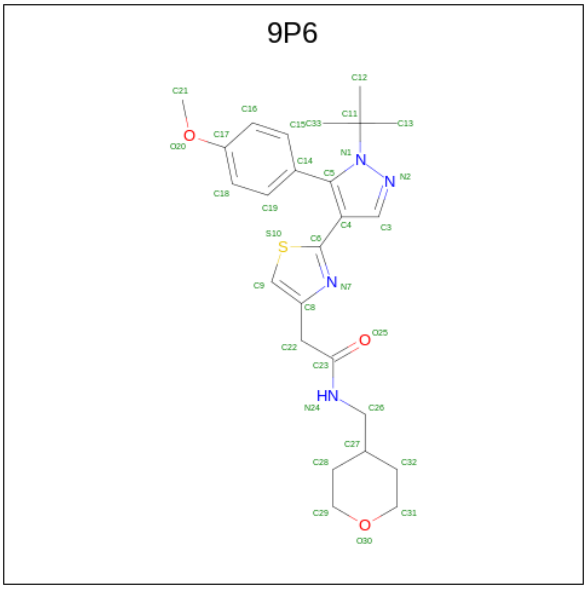
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	ALA	LYS	engineered mutation	UNP P51449
A	473	ALA	ARG	engineered mutation	UNP P51449
C	469	ALA	LYS	engineered mutation	UNP P51449
C	473	ALA	ARG	engineered mutation	UNP P51449
E	469	ALA	LYS	engineered mutation	UNP P51449
E	473	ALA	ARG	engineered mutation	UNP P51449
G	469	ALA	LYS	engineered mutation	UNP P51449
G	473	ALA	ARG	engineered mutation	UNP P51449

- Molecule 2 is a protein called Nuclear receptor corepressor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	S	0	0	0
			110	69	20	19	2			
2	D	12	Total	C	N	O	S	0	0	0
			87	56	16	14	1			
2	F	12	Total	C	N	O	S	0	0	0
			87	56	16	14	1			
2	H	15	Total	C	N	O	S	0	0	0
			108	68	20	18	2			

- Molecule 3 is 2-[2-[1- {tert}-butyl-5-(4-methoxyphenyl)pyrazol-4-yl]-1,3-thiazol-4-yl]- {N}-(oxan-4-ylmethyl)ethanamide (three-letter code: 9P6) (formula: $C_{25}H_{32}N_4O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			33	25	4	3	1		
3	C	1	Total	C	N	O	S	0	0
			33	25	4	3	1		
3	E	1	Total	C	N	O	S	0	0
			33	25	4	3	1		
3	G	1	Total	C	N	O	S	0	0
			33	25	4	3	1		

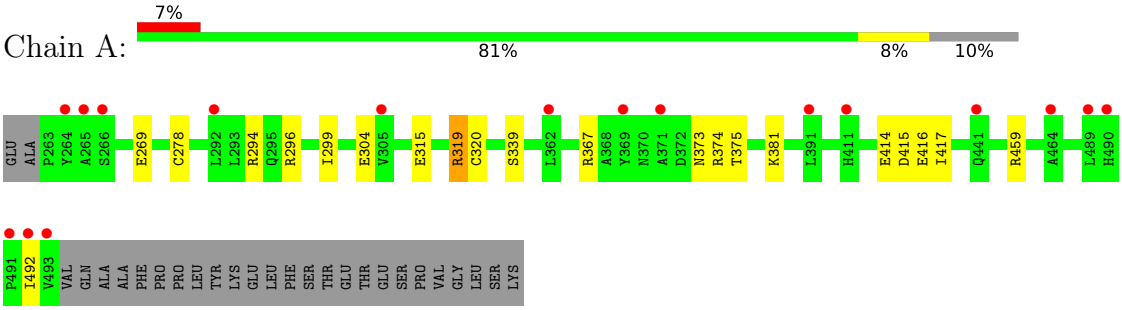
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	1	Total	O	0	0
			1	1		
4	C	27	Total	O	0	0
			27	27		
4	E	27	Total	O	0	0
			27	27		
4	F	1	Total	O	0	0
			1	1		
4	G	17	Total	O	0	0
			17	17		

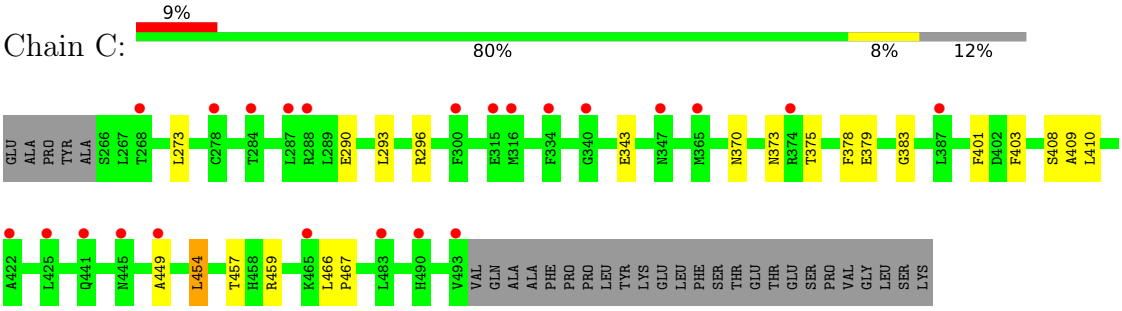
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

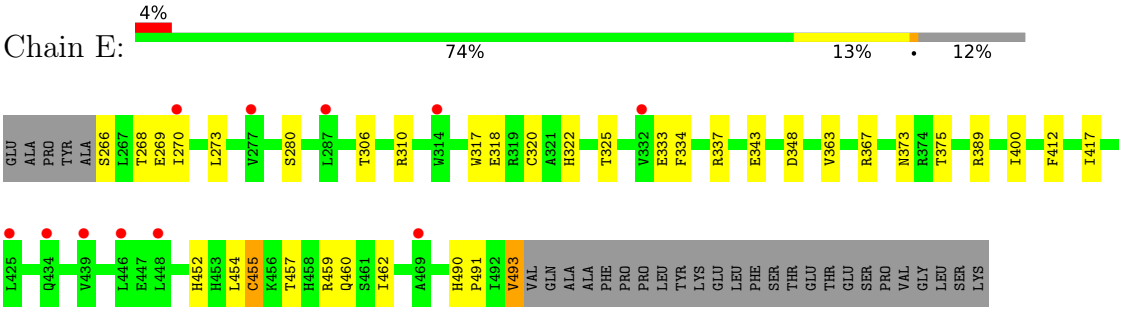
• Molecule 1: Nuclear receptor ROR-gamma



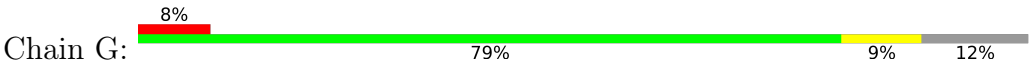
• Molecule 1: Nuclear receptor ROR-gamma

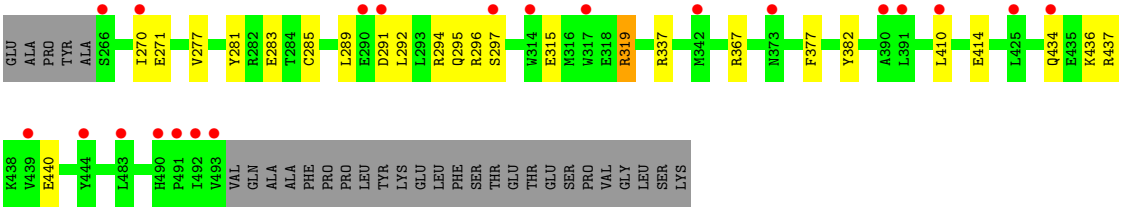


• Molecule 1: Nuclear receptor ROR-gamma

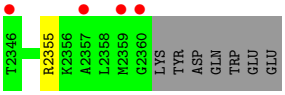


• Molecule 1: Nuclear receptor ROR-gamma

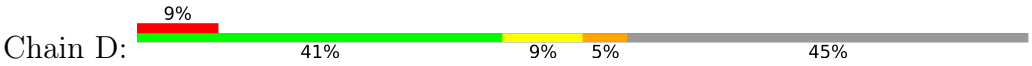


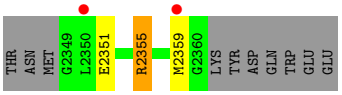


• Molecule 2: Nuclear receptor corepressor 2

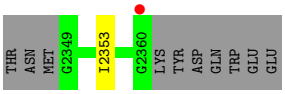


• Molecule 2: Nuclear receptor corepressor 2

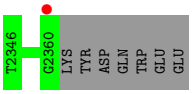




• Molecule 2: Nuclear receptor corepressor 2



• Molecule 2: Nuclear receptor corepressor 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.93Å 73.28Å 100.20Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	77.93 – 2.55 77.93 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.3 (77.93-2.55) 99.7 (77.93-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.217 , 0.243 0.227 , 0.250	Depositor DCC
R_{free} test set	1900 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	62.8	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.078 for h,-k,-l	Xtriage
Reported twinning fraction	0.540 for H, K, L 0.460 for -h,-k,l	Depositor
Outliers	0 of 36999 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8079	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 9P6

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.75	2/1927 (0.1%)	0.77	1/2596 (0.0%)
1	C	0.83	5/1894 (0.3%)	0.89	6/2550 (0.2%)
1	E	1.22	24/1902 (1.3%)	1.08	6/2562 (0.2%)
1	G	0.80	4/1895 (0.2%)	0.81	1/2552 (0.0%)
2	B	1.30	2/109 (1.8%)	0.99	0/143
2	D	1.64	2/86 (2.3%)	1.23	0/112
2	F	0.49	0/86	0.65	0/112
2	H	0.50	0/107	0.72	0/140
All	All	0.93	39/8006 (0.5%)	0.89	14/10767 (0.1%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	389	ARG	CZ-NH2	15.94	1.53	1.33
1	E	333	GLU	CD-OE1	14.07	1.41	1.25
1	E	333	GLU	CD-OE2	-12.10	1.12	1.25
1	C	379	GLU	CD-OE2	10.57	1.37	1.25
1	C	379	GLU	CG-CD	-10.39	1.36	1.51
1	E	334	PHE	CG-CD1	8.68	1.51	1.38
1	E	455	CYS	N-CA	8.34	1.63	1.46
1	C	408	SER	CA-CB	8.13	1.65	1.52
1	C	409	ALA	C-O	-7.63	1.08	1.23
1	E	389	ARG	CZ-NH1	7.33	1.42	1.33
1	G	367	ARG	CZ-NH1	7.11	1.42	1.33
2	D	2355	ARG	CZ-NH2	7.10	1.42	1.33
1	E	459	ARG	CZ-NH2	7.07	1.42	1.33
1	E	334	PHE	CD1-CE1	-7.02	1.25	1.39
1	G	319	ARG	CZ-NH2	7.02	1.42	1.33
1	G	319	ARG	CZ-NH1	7.01	1.42	1.33
2	B	2355	ARG	CZ-NH1	7.01	1.42	1.33
1	A	319	ARG	CZ-NH2	7.01	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2355	ARG	CZ-NH2	6.99	1.42	1.33
1	A	319	ARG	CZ-NH1	6.95	1.42	1.33
1	G	367	ARG	CZ-NH2	6.93	1.42	1.33
2	D	2355	ARG	CZ-NH1	6.91	1.42	1.33
1	E	270	ILE	C-O	-6.81	1.10	1.23
1	E	459	ARG	CZ-NH1	6.81	1.41	1.33
1	E	363	VAL	CB-CG1	6.25	1.66	1.52
1	C	401	PHE	CE2-CZ	-6.18	1.25	1.37
1	E	452	HIS	C-O	5.82	1.34	1.23
1	E	317	TRP	C-N	-5.77	1.20	1.34
1	E	268	THR	C-O	-5.53	1.12	1.23
1	E	334	PHE	N-CA	5.41	1.57	1.46
1	E	273	LEU	N-CA	5.40	1.57	1.46
1	E	462	ILE	CA-C	5.29	1.66	1.52
1	E	320	CYS	C-N	5.17	1.46	1.34
1	E	452	HIS	CB-CG	5.16	1.59	1.50
1	E	322	HIS	CA-C	5.11	1.66	1.52
1	E	454	LEU	C-N	-5.09	1.22	1.34
1	E	363	VAL	CA-CB	-5.08	1.44	1.54
1	E	493	VAL	N-CA	5.06	1.56	1.46
1	E	400	ILE	CA-CB	-5.01	1.43	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	389	ARG	NE-CZ-NH2	-21.21	109.69	120.30
1	E	389	ARG	NE-CZ-NH1	15.07	127.84	120.30
1	C	378	PHE	CB-CG-CD1	-11.12	113.02	120.80
1	C	401	PHE	CB-CG-CD2	8.27	126.59	120.80
1	E	334	PHE	CB-CG-CD1	6.27	125.19	120.80
1	C	378	PHE	CG-CD1-CE1	-6.12	114.06	120.80
1	C	401	PHE	CG-CD2-CE2	5.80	127.18	120.80
1	G	367	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	C	378	PHE	CZ-CE2-CD2	-5.65	113.31	120.10
1	E	322	HIS	N-CA-CB	5.58	120.65	110.60
1	C	378	PHE	CD1-CG-CD2	5.50	125.45	118.30
1	E	348	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	294	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	E	348	ASP	CB-CG-OD1	-5.15	113.67	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1887	0	1881	11	1
1	C	1856	0	1851	17	0
1	E	1864	0	1860	14	0
1	G	1857	0	1855	15	0
2	B	110	0	122	0	0
2	D	87	0	100	2	0
2	F	87	0	100	1	0
2	H	108	0	117	0	0
3	A	33	0	0	1	0
3	C	33	0	0	0	0
3	E	33	0	0	1	0
3	G	33	0	0	1	0
4	A	18	0	0	2	0
4	B	1	0	0	0	0
4	C	27	0	0	1	0
4	E	27	0	0	0	0
4	F	1	0	0	0	0
4	G	17	0	0	2	0
All	All	8079	0	7886	60	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:LEU:HD12	1:C:467:PRO:HD2	1.21	1.12
1:C:466:LEU:CD1	1:C:467:PRO:HD2	2.04	0.86
1:C:466:LEU:HD12	1:C:467:PRO:CD	2.08	0.82
1:A:367:ARG:HD3	1:A:417:ILE:HG12	1.73	0.71
1:C:457:THR:HG23	1:C:459:ARG:HB2	1.71	0.71
1:C:403:PHE:CD1	1:C:467:PRO:HG2	2.31	0.65
1:A:320:CYS:HB3	3:A:9000:9P6:N2	2.17	0.59
1:G:291:ASP:O	1:G:295:GLN:HG2	2.05	0.56
1:C:454:LEU:HA	1:C:457:THR:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:ARG:HG2	1:C:459:ARG:HH11	1.73	0.54
1:G:410:LEU:N	1:G:410:LEU:HD23	2.22	0.54
1:C:403:PHE:CE1	1:C:467:PRO:HG2	2.43	0.54
3:E:9000:9P6:C14	3:E:9000:9P6:C13	2.86	0.54
3:G:9000:9P6:C14	3:G:9000:9P6:C12	2.89	0.51
1:G:283:GLU:OE2	1:G:337:ARG:NH1	2.44	0.51
1:E:318:GLU:OE1	1:E:493:VAL:HG13	2.10	0.51
1:E:455:CYS:HA	1:E:460:GLN:NE2	2.26	0.51
1:E:457:THR:HG22	1:G:297:SER:O	2.12	0.50
1:C:375:THR:HG1	1:C:383:GLY:C	2.15	0.50
1:G:315:GLU:O	1:G:319:ARG:HG3	2.12	0.49
1:A:492:ILE:HG13	4:A:9104:HOH:O	2.11	0.49
1:A:315:GLU:O	1:A:319:ARG:HG3	2.13	0.49
1:E:266:SER:HB2	1:E:269:GLU:HB2	1.95	0.49
1:E:325:THR:HG22	2:F:2353:ILE:HD13	1.94	0.49
1:E:266:SER:HB2	1:E:269:GLU:CG	2.43	0.48
1:G:289:LEU:HD22	1:G:414:GLU:HG2	1.95	0.48
1:A:339:SER:N	4:A:9101:HOH:O	2.44	0.48
1:E:490:HIS:HB3	1:E:491:PRO:HD2	1.95	0.48
1:G:434:GLN:O	1:G:436:LYS:HE3	2.13	0.48
1:C:457:THR:CG2	1:C:459:ARG:HB2	2.42	0.48
1:E:367:ARG:HD3	1:E:417:ILE:HG13	1.94	0.48
1:G:294:ARG:NE	1:G:294:ARG:HA	2.29	0.47
1:G:296:ARG:HG2	1:G:382:TYR:CZ	2.49	0.47
1:G:281:TYR:CE2	1:G:285:CYS:SG	3.09	0.46
1:C:410:LEU:O	1:C:459:ARG:NH2	2.40	0.45
1:A:304:GLU:OE1	1:A:381:LYS:NZ	2.49	0.45
1:A:296:ARG:O	1:A:299:ILE:HD11	2.17	0.45
1:E:306[A]:THR:O	1:E:310:ARG:HG3	2.16	0.45
1:A:278[A]:CYS:SG	1:A:415:ASP:CG	2.96	0.43
1:G:377:PHE:O	4:G:9101:HOH:O	2.21	0.43
1:C:370:ASN:ND2	4:C:9101:HOH:O	2.08	0.43
1:G:277:VAL:HG22	4:G:9107:HOH:O	2.18	0.43
1:G:437:ARG:HA	1:G:440:GLU:HG2	2.00	0.43
1:C:373:ASN:OD1	1:C:375:THR:HG22	2.19	0.43
1:A:416:GLU:OE2	1:A:459:ARG:HD3	2.18	0.42
2:D:2359:MET:HA	2:D:2359:MET:CE	2.48	0.42
1:E:280:SER:OG	1:E:337:ARG:HB3	2.18	0.42
1:E:318:GLU:OE2	1:E:318:GLU:HA	2.19	0.42
1:G:270:ILE:CG1	1:G:271:GLU:N	2.81	0.42
1:C:343:GLU:N	1:C:343:GLU:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:ASN:O	1:E:375:THR:HG23	2.20	0.42
1:A:414:GLU:OE2	1:A:414:GLU:HA	2.20	0.41
1:C:454:LEU:HA	1:C:454:LEU:HD12	1.85	0.41
1:A:373:ASN:O	1:A:375:THR:HG23	2.20	0.41
1:C:273:LEU:HD23	1:C:449:ALA:HB2	2.02	0.41
1:C:293:LEU:HA	1:C:296:ARG:HD2	2.02	0.41
1:E:343:GLU:OE1	1:E:343:GLU:N	2.54	0.41
2:D:2351:GLU:OE2	2:D:2355:ARG:NH2	2.50	0.41
1:G:292:LEU:HD22	1:G:377:PHE:CD1	2.56	0.40
1:E:412:PHE:HB3	1:E:417:ILE:HG12	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLU:OE2	1:A:374:ARG:NH1[2_756]	2.06	0.14

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/258 (89%)	228 (99%)	2 (1%)	0	100	100
1	C	226/258 (88%)	224 (99%)	2 (1%)	0	100	100
1	E	227/258 (88%)	224 (99%)	3 (1%)	0	100	100
1	G	226/258 (88%)	223 (99%)	3 (1%)	0	100	100
2	B	13/22 (59%)	12 (92%)	1 (8%)	0	100	100
2	D	10/22 (46%)	10 (100%)	0	0	100	100
2	F	10/22 (46%)	10 (100%)	0	0	100	100
2	H	13/22 (59%)	13 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	955/1120 (85%)	944 (99%)	11 (1%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	206/228 (90%)	206 (100%)	0	100 100
1	C	203/228 (89%)	201 (99%)	2 (1%)	76 84
1	E	204/228 (90%)	204 (100%)	0	100 100
1	G	203/228 (89%)	203 (100%)	0	100 100
2	B	11/18 (61%)	11 (100%)	0	100 100
2	D	8/18 (44%)	8 (100%)	0	100 100
2	F	8/18 (44%)	8 (100%)	0	100 100
2	H	10/18 (56%)	10 (100%)	0	100 100
All	All	853/984 (87%)	851 (100%)	2 (0%)	93 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	290	GLU
1	C	454	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	453	HIS
1	C	322	HIS
1	C	411	HIS
1	E	286	GLN
1	G	411	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	9P6	G	9000	-	30,36,36	0.93	3 (10%)	33,51,51	1.44	3 (9%)
3	9P6	A	9000	-	30,36,36	0.90	1 (3%)	33,51,51	1.52	1 (3%)
3	9P6	C	9000	-	30,36,36	0.85	1 (3%)	33,51,51	1.41	2 (6%)
3	9P6	E	9000	-	30,36,36	0.93	1 (3%)	33,51,51	1.46	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	9P6	G	9000	-	-	6/19/33/33	0/4/4/4
3	9P6	A	9000	-	-	7/19/33/33	0/4/4/4
3	9P6	C	9000	-	-	6/19/33/33	0/4/4/4
3	9P6	E	9000	-	-	6/19/33/33	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	9000	9P6	C6-S10	-2.22	1.70	1.73
3	E	9000	9P6	C6-S10	-2.18	1.70	1.73
3	G	9000	9P6	C22-C8	-2.11	1.49	1.51
3	G	9000	9P6	C6-S10	-2.08	1.70	1.73
3	C	9000	9P6	C23-N24	2.03	1.38	1.33
3	G	9000	9P6	C23-N24	2.03	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	9000	9P6	C4-C5-N1	-7.36	104.58	108.92
3	E	9000	9P6	C4-C5-N1	-6.60	105.03	108.92
3	G	9000	9P6	C4-C5-N1	-6.55	105.05	108.92
3	C	9000	9P6	C4-C5-N1	-6.17	105.28	108.92
3	E	9000	9P6	C33-C11-C12	-2.49	105.53	110.05
3	C	9000	9P6	C33-C11-C13	-2.43	105.64	110.05
3	G	9000	9P6	C14-C5-N1	2.30	126.83	123.38
3	G	9000	9P6	C33-C11-C13	-2.01	106.40	110.05

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	9000	9P6	N24-C26-C27-C32
3	E	9000	9P6	C15-C14-C5-N1
3	E	9000	9P6	C19-C14-C5-N1
3	G	9000	9P6	C15-C14-C5-N1
3	G	9000	9P6	C19-C14-C5-N1
3	G	9000	9P6	C16-C17-O20-C21
3	G	9000	9P6	C18-C17-O20-C21
3	C	9000	9P6	C16-C17-O20-C21
3	C	9000	9P6	C18-C17-O20-C21
3	E	9000	9P6	C16-C17-O20-C21
3	E	9000	9P6	C18-C17-O20-C21
3	A	9000	9P6	C16-C17-O20-C21
3	A	9000	9P6	C18-C17-O20-C21
3	G	9000	9P6	C15-C14-C5-C4
3	E	9000	9P6	C19-C14-C5-C4
3	A	9000	9P6	C15-C14-C5-N1
3	C	9000	9P6	C15-C14-C5-N1
3	C	9000	9P6	C19-C14-C5-N1

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Mol	Chain	Res	Type	Atoms
3	E	9000	9P6	C15-C14-C5-C4
3	G	9000	9P6	C19-C14-C5-C4
3	A	9000	9P6	C19-C14-C5-N1
3	A	9000	9P6	C15-C14-C5-C4
3	C	9000	9P6	C15-C14-C5-C4
3	A	9000	9P6	C19-C14-C5-C4
3	C	9000	9P6	C19-C14-C5-C4

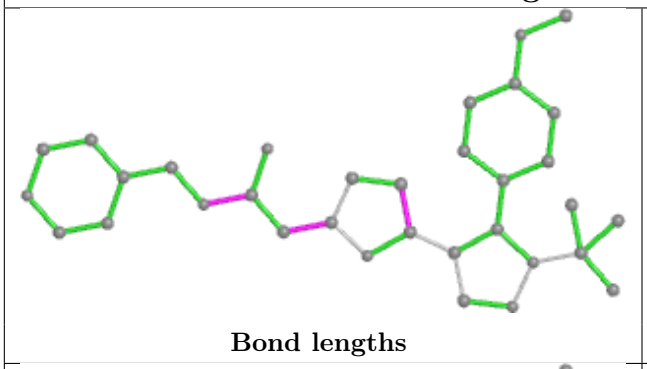
There are no ring outliers.

3 monomers are involved in 3 short contacts:

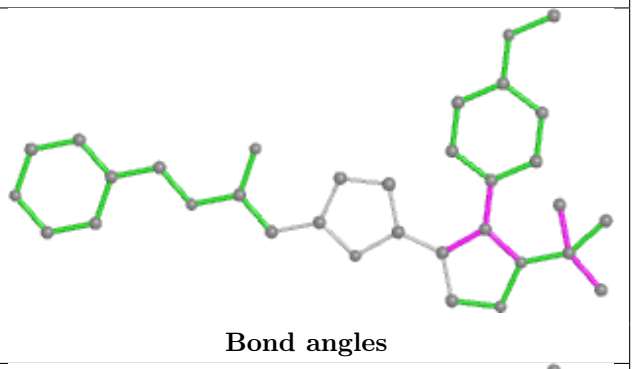
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	9000	9P6	1	0
3	A	9000	9P6	1	0
3	E	9000	9P6	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

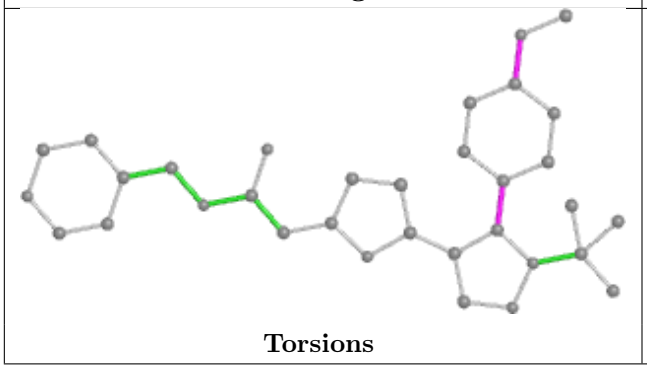
Ligand 9P6 G 9000



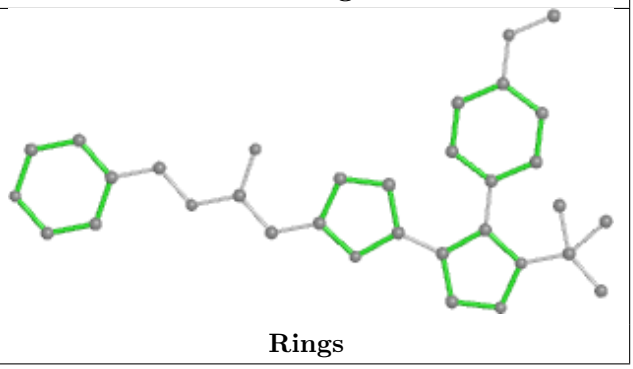
Bond lengths



Bond angles

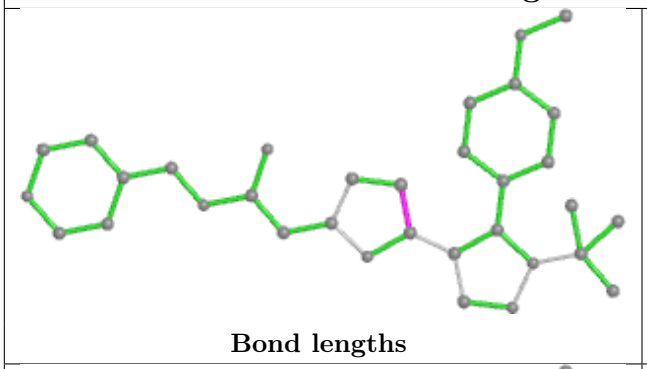


Torsions

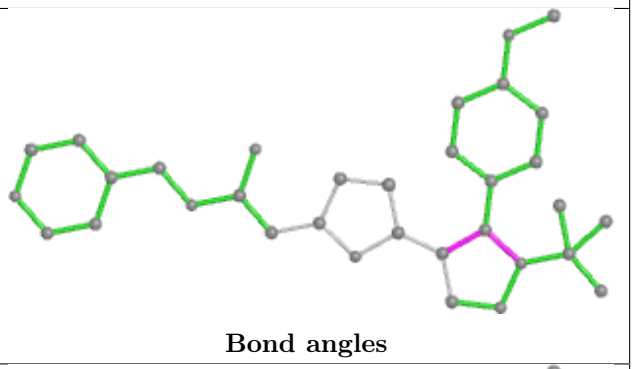


Rings

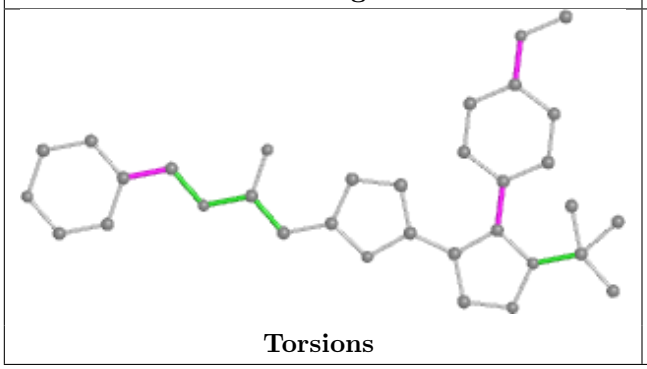
Ligand 9P6 A 9000



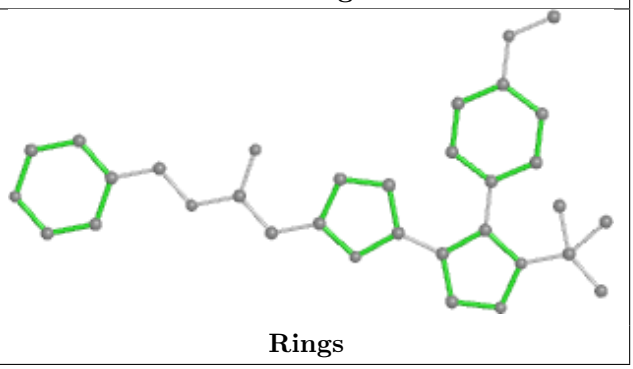
Bond lengths



Bond angles

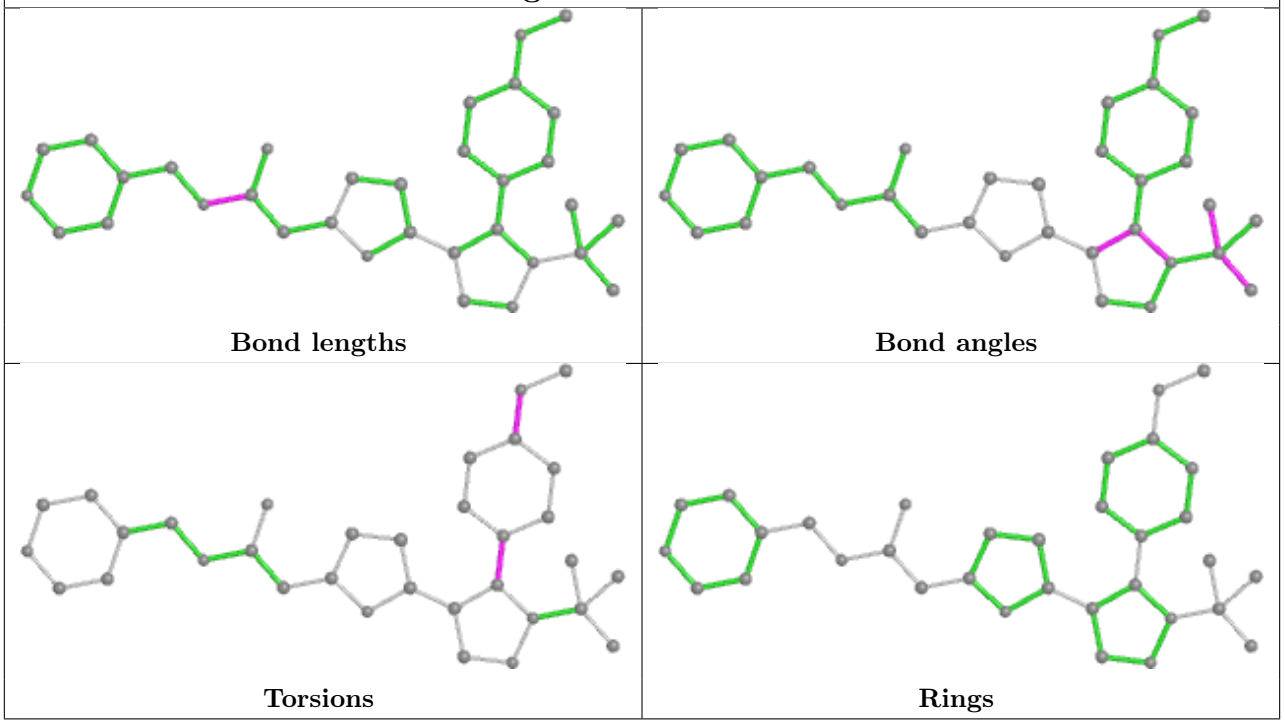


Torsions

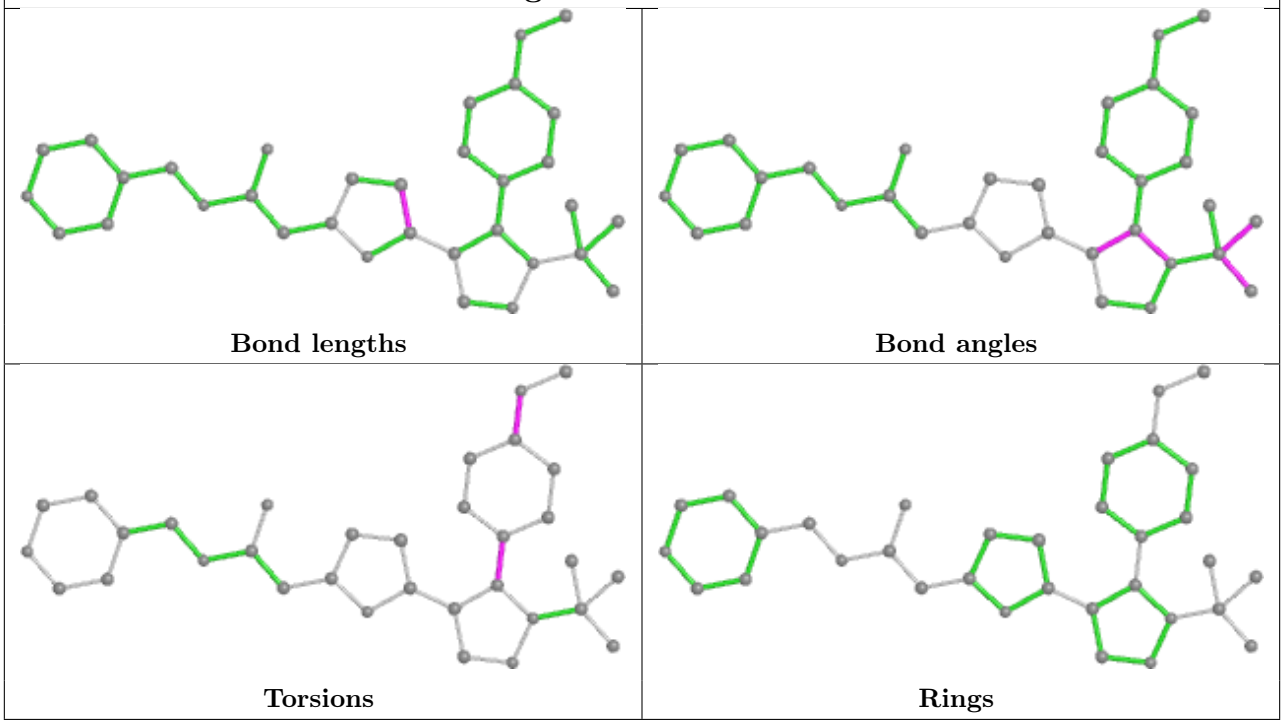


Rings

Ligand 9P6 C 9000



Ligand 9P6 E 9000



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	231/258 (89%)	0.64	17 (7%) 14 18	37, 59, 96, 131	0
1	C	228/258 (88%)	0.78	23 (10%) 7 8	39, 65, 101, 145	0
1	E	228/258 (88%)	0.53	11 (4%) 30 37	35, 58, 87, 103	0
1	G	228/258 (88%)	0.66	21 (9%) 9 10	33, 64, 99, 138	0
2	B	15/22 (68%)	1.23	4 (26%) 0 0	59, 70, 118, 119	0
2	D	12/22 (54%)	1.22	2 (16%) 1 1	72, 85, 107, 140	0
2	F	12/22 (54%)	0.70	1 (8%) 11 13	59, 73, 91, 101	0
2	H	15/22 (68%)	0.63	1 (6%) 17 21	57, 67, 89, 97	0
All	All	969/1120 (86%)	0.67	80 (8%) 11 13	33, 63, 99, 145	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	491	PRO	6.4
1	C	288	ARG	6.3
1	A	264	TYR	5.5
1	E	287	LEU	4.9
2	D	2359	MET	4.5
1	A	265	ALA	4.2
2	D	2350	LEU	4.1
1	G	270	ILE	4.0
1	A	266	SER	3.9
1	G	434	GLN	3.9
1	G	266	SER	3.8
1	C	316	MET	3.7
1	G	297	SER	3.7
2	B	2346	THR	3.6
1	G	490	HIS	3.4
2	B	2360	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	490	HIS	3.4
1	C	445	ASN	3.3
1	C	365	MET	3.3
1	A	493	VAL	3.1
1	G	342	MET	3.1
1	E	270	ILE	3.1
1	C	387	LEU	3.0
1	A	490	HIS	2.9
1	E	439	VAL	2.8
1	C	334	PHE	2.8
1	C	425	LEU	2.8
1	A	492	ILE	2.8
2	B	2357	ALA	2.8
1	G	373	ASN	2.8
2	B	2359	MET	2.8
1	E	277	VAL	2.7
1	G	410	LEU	2.7
1	C	422	ALA	2.7
2	H	2360	GLY	2.7
1	C	284	THR	2.6
1	C	287	LEU	2.6
1	C	268	THR	2.6
1	C	315	GLU	2.5
1	G	314	TRP	2.5
1	E	448	LEU	2.4
1	C	441	GLN	2.4
1	G	483	LEU	2.4
1	C	278	CYS	2.4
1	E	314	TRP	2.4
1	E	425	LEU	2.4
1	E	332	VAL	2.4
1	C	340	GLY	2.3
2	F	2360	GLY	2.3
1	C	483	LEU	2.3
1	A	491	PRO	2.3
1	A	369	TYR	2.3
1	G	425	LEU	2.3
1	G	290	GLU	2.3
1	C	493	VAL	2.3
1	A	292	LEU	2.2
1	A	441	GLN	2.2
1	A	305	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	439	VAL	2.2
1	C	449	ALA	2.2
1	C	347	ASN	2.2
1	G	444	TYR	2.2
1	A	411	HIS	2.2
1	E	469	ALA	2.2
1	G	390	ALA	2.2
1	C	300	PHE	2.1
1	A	391	LEU	2.1
1	E	434	GLN	2.1
1	A	371	ALA	2.1
1	A	362	LEU	2.1
1	E	446	LEU	2.1
1	G	317	TRP	2.1
1	G	391	LEU	2.1
1	C	374	ARG	2.1
1	G	492	ILE	2.1
1	G	291	ASP	2.0
1	C	465	LYS	2.0
1	A	464	ALA	2.0
1	G	493	VAL	2.0
1	A	489	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	9P6	C	9000	33/33	0.89	0.23	36,65,76,81	0

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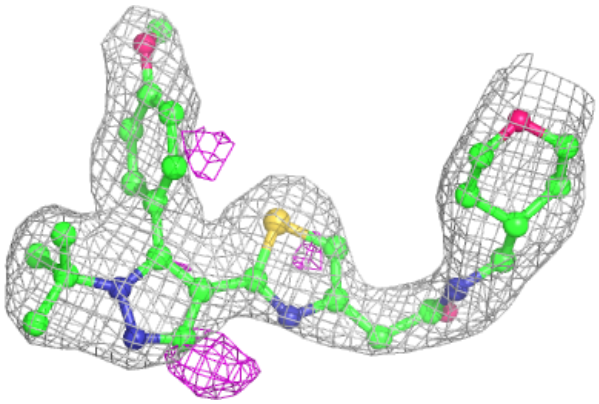
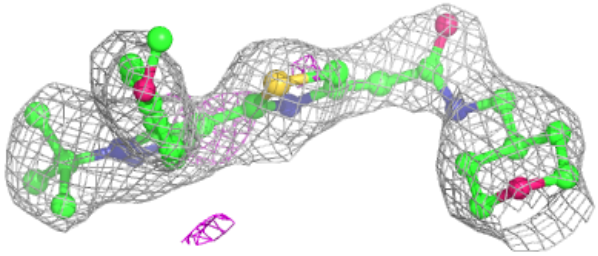
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	9P6	A	9000	33/33	0.94	0.23	31,55,68,73	0
3	9P6	E	9000	33/33	0.95	0.24	31,44,57,72	0
3	9P6	G	9000	33/33	0.95	0.20	30,46,78,83	0

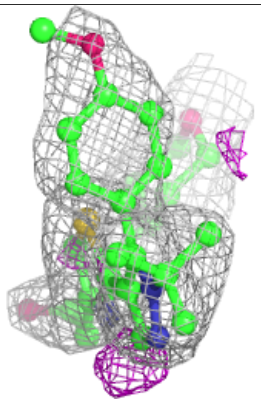
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 9P6 C 9000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

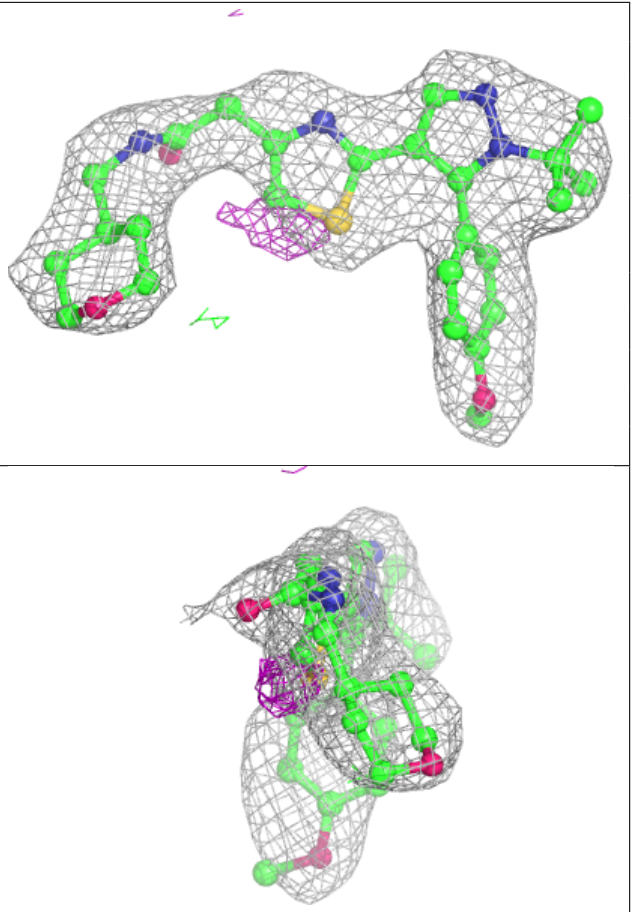






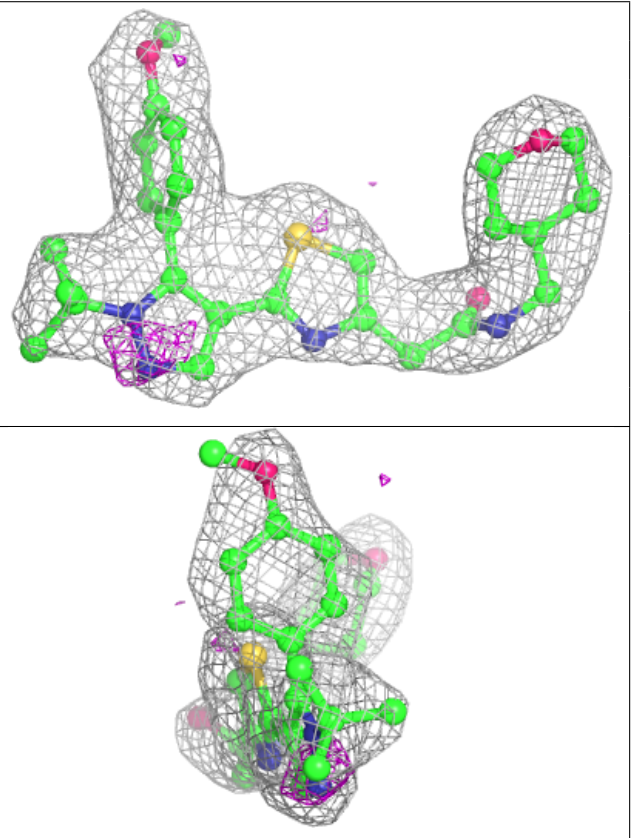
Electron density around 9P6 A 9000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



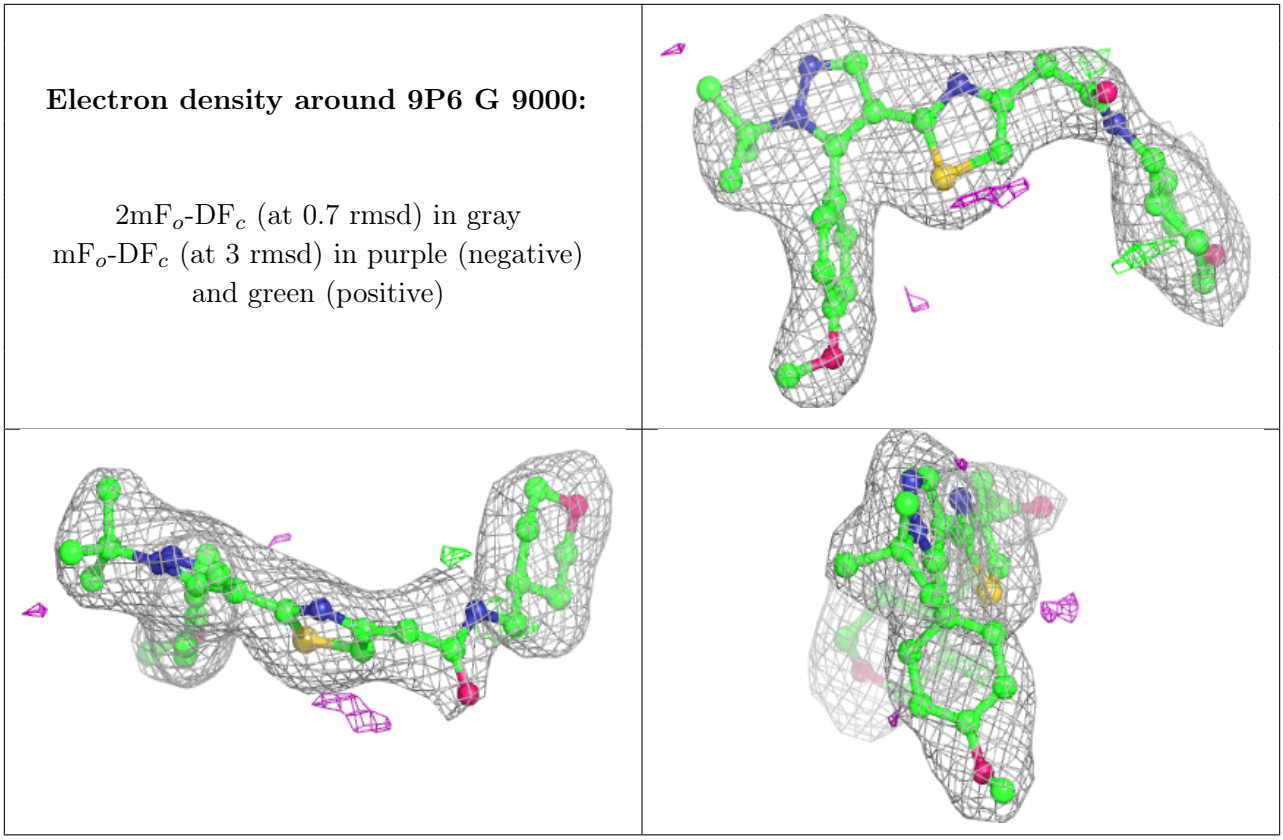
Electron density around 9P6 E 9000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 9P6 G 9000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.